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On the calculation of vibrational-vibrational rates of CO_2[1] JESPER JANSSEN, JAN VAN DIJK, JOS SUIJKER, Eindhoven University of Technology — The increase of the CO_2 concentration in the air and the accompanying climate change has driven the need to limit the CO_2 output. One of the possible ways is to convert CO_2 back into fossil fuels using plasmas. The conversion of CO_2 to CO is a crucial step. The most energy efficient path to dissociation uses vibrational pumping. The vibrational-vibrational reactions are poorly understood. Numerical models use empirical scaling relations whose accuracy is unknown. The aim of this project is to calculate the vibrational-vibrational rates. The number of dimensions of the system is too large to calculate the potential energy surface using ab initio methods for all possible orientations. Therefore an analytical potential surface is constructed based on Zúñiga et al and Bartolomei et al. This potential is used to evaluate several trajectories of two colliding CO_2 molecules. By varying the initial conditions and by sampling several trajectories, the reaction rates can be deduced. In a later stage of the project the improved reaction rates will be used to simulate the microwave reactor using PLASIMO. This model will couple equations for momentum, continuity, Te, Th and electromagnetics self-consistently. The model will be used to optimize the reactor.

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